STATIC AND DYNAMIC CONTACT ANGLES – A PHASE FIELD MODELLING

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Recently we proposed a phase field model for Marangoni convection in compressible fluids of van der Waals type far from criticality. The phase field models introduce an order parameter to the usual set of state variables in order to provide an explicit indication of the thermodynamic phase in each point of the system. We choose the fluid density ρ as phase field function. So $\rho = 1$ designates the liquid phase and $\rho = 0$ the vapor bulk. With the help of the phase variable ρ, all the system parameters can be expressed as functions varying continuously from one medium to the other. Therefore, the problem is treated like an entire one phase problem and the interface conditions are substituted by some extra−terms in the Navier−Stokes equation. The theoretical description is based on the Navier−Stokes equation with extra phase field terms

$$\rho \frac{d\vec{v}}{dt} = -\nabla p + \rho \nabla \left(\nabla \cdot (\mathcal{K} \nabla \rho) \right) + \nabla \cdot (\eta \nabla \vec{v}) + \nabla (\lambda \nabla \cdot \vec{v}) + \rho \vec{g} \qquad \lambda \approx \frac{\eta}{3}.$$

the classical heat equation

$$\rho c \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T)$$

and the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0.$$

The model previously developed for two−layer geometry [1−4] is extended in this paper to drops and bubbles. We solve the problem numerically, starting from an initial noise density. A randomly distributed initial density may act as *seeds* for phase separation in the van der Waals fluid. In the later, drops or bubbles are found by *nucleation* and *coarsening*. The system evolves to drops in a vapor atmosphere or bubbles in a liquid, depending on the total mass.

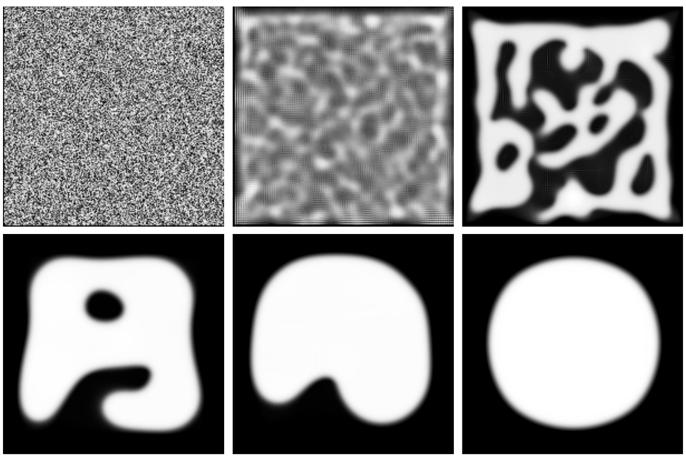

Figure 1: *Drop formation in a vapor atmosphere under microgravity conditions.*

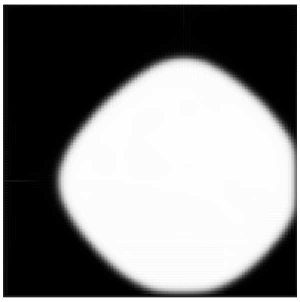

Figure 2: *The boundary conditions for the density field at the solid walls may favour the drop to be in contact with the solid surface.*

Figure 1 displays time series in (x, z) plane for the formation of a liquid drop in a vapor atmosphere for an isothermal system without gravity.

The boundary conditions for the density field at the solid walls play an important role for the contact angle at the solid surface and determine the position of the droplet. In our model we control the contact angle through the density at the solid boundary ρ_S [5]. L. Pismen *et al.* showed that, for solid−fluid interactions short ranged compared to the thickness of the diffuse vapor−liquid interface, the only condition enforced on the solid surface is

$$\rho = \rho_S.$$

Starting from the Young−Laplace relation, for the stresses balance on the contact line, an analytical relation between the static contact angle and the solid density ρ_S is established [5]:

$$\cos\theta = -1 + 6\,\rho_S^2 - 4\,\rho_S^3. \tag{1}$$

Thus, for $\rho_s = 0$ the liquid drop will be pushed away from all the four walls and, after a while, a single liquid droplet will be obtained in the middle of the box ("no−wetting" case illustrated in Figure 1). For $\rho_S \neq 0$ the drop is attracted to the wall, the boundary conditions favour now the droplet to be in contact with the solid surface (see Figure 2 for $\rho_s = 0.1$). The situation illustrated in Figure 2 corresponds to a "partial wetting" case. Our aim is to compare quantitatively the phase field simulations with the analytical formula (1), to adjust the phase field model for drop motion on inclined substrate under gravity effects and to investigate the dynamic contact angles of a spreading droplet at different velocities of the contact line.

References

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